FINAL REPORT

for

CONTINUATION OF LOW-ALTITUDE SATELLITE INTERACTION PROBLEM INVESTIGATION
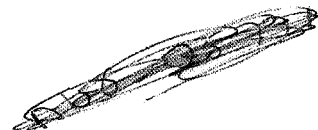
Contract No. NAS5-11145

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for

Goddard Space Flight Center
National Aeronautics and Space Administration
Greenbelt, Maryland

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PREFACE

This is the final report on the Continuation of Low-Altitude
Satellite Interaction Problem Investigation. The study was con-
ducted by the Astro-Electronics Division of RCA for the National
Aeronautics and Space Administration under Contract No. NAS5-
11145. Work on the study was accomplished during the period
from May 28, 1968 through April 28, 1969. This report is
identified as GSFC Report No. CR94922.

SUMMARY

It is well-known that many of the important aeronomic processes and reactions that directly affect the structure of the upper atmosphere occur in the altitude range of about 90 to 150 kilometers. The desirability of extensive aeronomic measurements in this region points to the necessity of using data from rapidly moving vehicles such as sounding rockets and satellites having low perigees. A typically sized body passing through this altitude region disturbs the atmospheric gas particles before their arrival at the measuring instrument in the body, which precludes the use of free-molecular theory for data interpretation. Because the typical body size is comparable to the mean free path of the gas particles throughout much of this region, ordinary continuum fluid theory is likewise inapplicable. Accordingly, this altitude regime is generally referred to as the "transition region".

In the preceding study (Contract No. NAS5-11016), a numerical program was developed, based upon a direct simulation Monte Carlo technique as first utilized by G. A. Bird. The feasibility of the Monte Carlo technique was established, and the flow field was computed for a two-gas mixture for the case of a sphere and for an infinite cylinder where axis was perpendicular to the direction of free stream flow. A separate program was required for each different body geometry and no attempt had been made to provide separate sub-routines to simplify the programming procedures for varying the field parameters. The present study was undertaken to generally reorganize and expand the earlier programs. The major results specifically produced by this study are as follows:

(1) The previous two-dimensional two-fluid program was reorganized and generalized to improve its efficiency, flexibility, and usefulness. A single program can now accommodate any axi-symmetric body composed of a finite number of connected quadric surfaces.

(2) The program was extended to more general situations which included examining the feasibility of a three-dimensional, multiple-fluid case. (Programming for this case has also commenced.)

(3) A three-dimensional program was constructed for computing internal flow conditions in a body cavity and relating the internal flow to the actual surface conditions predicted by the two-dimensional external flow program.

(4) Techniques were examined for synthesizing a composite gas when more than two species must be considered.

This report describes in detail the Monte Carlo procedure and the preceding results. The formal documentation for the two-dimensional, two-fluid program has been provided to NASA under separate cover.

This study demonstrated the feasibility of generalizing the programs; of constructing an operational three-dimensional program; of coupling external and internal flow programs; and of simulating the effects of two or more gases by a single composite gas.

A number of production runs were accomplished for a spherical body. This shape was selected mainly because a limited amount of data from the earlier program was available for comparison.

Based upon the results of this study, the following investigations are recommended:

(1) Develop an operational generalized three-dimensional, two-fluid program.

(2) Couple the external body flow distribution obtained from the three-dimensional program with the internal flow program.

(3) Make physical interpretations of the program results based upon a detailed study of the data.

(4) Determine the actual flow characteristics for a specific spacecraft configuration and altitude regime.

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SECTION I

INTRODUCTION

Many of the physical and chemical processes which determine the properties of the earth's atmosphere occur in the region of approximately 90 to 150 kilometers; for example, absorption of solar extreme ultraviolet radiation by the neutral atmosphere. To date these processes are not all completely understood so that further exploration is necessary, especially to acquire information on composition and density in this altitude region. However, making such measurements creates a two-fold problem.

First, the region is directly accessible only to sounding rockets and satellites. Sounding rocket measurements are limited to single, localized vertical profiles, and satellite programs have been extremely limited in this altitude region. (NASA is planning an aeronomy explorer program in the near future.)

The second part of the problem, the one which this study addresses, is the interaction of the measurement vehicle with the atmosphere. A measuring instrument mounted on a high speed (superthermal) spacecraft does not "see" the true undisturbed environment, but rather, the environment modified by the presence of the spacecraft. The purpose of this study is to develop a theoretical technique for calculating these interaction effects under a variety of conditions.

The altitudes from about 90 to 150 kilometers are referred to as the "transition region" for the following reason. Below 90 kilometers, the atmosphere is sufficiently dense to permit fluid analysis by continuum theory. The mean free paths of the gas particles will be very much less than typical spacecraft dimensions. Above 150 kilometers, the mean free paths will be many times greater than the spacecraft dimensions, permitting the use of free molecular theory for predicting interaction effects. In the transition region, neither theory is generally applicable. As an approach to solving the problem, a numerical program was developed under Contract Number NAS5-11016, based on a direct simulation Monte Carlo technique. The technique as modified and utilized in this present study is described in detail in Section II, Theoretical Foundation, of this report. The first programs, under Contract No. NAS5-11016, predicted body flow conditions over a range of Knudsen numbers (the ratio of the mean free path to body size) for various number density ratios and mass ratios of a two-specie gas for an infinite cylinder (axis perpendicular to the free stream direction), and also provided some limited results for a spherical body.

The main physical results of these first programs were: (1) a notable increase in total particle flux at the stagnation point over the free stream value, and (2) a marked increase in the number ratio of the heavy-to-light species at the stagnation point. Other results were too tentative in nature (because of the small statistical sample sizes) to discuss here. The program was written in FORTRAN IV, and all computer runs were performed on the IBM 360-65.

These first programs were rather inefficient in terms of programming and computer running times and required separate programs for each body geometry. The programs applied to only simple, two-dimensional, two-fluid situations. As such, the programs served to verify the direct simulation Monte Carlo technique, but were not generally useful or amenable to examining real physical situations where geometry is not so idealized.

The present study is a direct outgrowth of the previous effort described in the preceding paragraph. The major research objectives of this study are discussed below.

A. THE TWO-DIMENSIONAL PROGRAM

One objective was to optimize the previous programs through reorganization, improved logic, and the introduction of separate sub-routines for each of the main sub-divisions of the programs.

A second objective was to generalize the body geometry sub-routine so that a single program would serve a variety of geometric shapes. The body reflection sub-routine was also generalized to permit varying the ratio of diffuse to specular reflections through a complete range. The revised generalized program can calculate particle-body interactions for any body whose axis of symmetry is parallel to the velocity vector (assumed to be the free stream direction), where the body is generated by rotating first- or second-order curves about the axis of symmetry, or a body having one very large dimension which is normal to the flow, such as a long cylinder or airfoil. The body can be composed of several different connected surfaces having a common symmetry axis.

B. THE GENERALIZED PROGRAM

The study required the extension of the program to situations more general than the two-dimensional, two-fluid case. The three-dimensional, two-fluid case was specifically examined for feasibility based on requirements for programming, computer storage, and computer running times. The program was determined feasible for computers with storage and speeds equal to or greater than the IBM 360-91, and programming for this case was started in this present study.

C.   INTERNAL FLOW PROGRAM

The objective here was to construct a program for measuring the flow conditions inside a body cavity and relate the flow distribution calculated by the external flow program to the internal flow. Because of the manner in which particles are sampled (each sample particle represents many thousands of actual particles), the sample sizes at any point on the body surface are rather small for a moderate computer running time. Thus, for cavities with relatively small openings, the flow rate through the entrance region is very low and the existing program takes a long time for the cavity to reach steady state. Techniques for reducing this computer time were investigated.

D.   COMPOSITE GAS AND TRACE GAS TECHNIQUES

Techniques were to be investigated for synthesizing a composite gas so that when more than two species are present (one may be a trace gas), the problem can be satisfactorily approximated as a two-gas mixture. (A three-fluid program requires 50 percent more computer storage space for particle information and would also require 2.25 more computational time for particle-particle collisions, than a comparable two-fluid program.) A nitrogen, molecular oxygen, and atomic oxygen composite was tested successfully.

E.   DOCUMENTATION

Documentation was to be prepared for the two-dimensional, two-fluid program.

SECTION II

THEORETICAL FOUNDATION

This study is concerned with the investigation of fluid motions on the basis of kinetic theory. Of primary interest is the flow field around bodies having dimensions generally similar to the mean-free-pathlength of the molecules themselves. The physical situation is that of the many-body problem where Liouville's Theorem provides the fundamental equation of motion; however, the simpler Boltzmann equation is adequate for the case of rarefied gases when higher order collisions are ignored (collisions which occur simultaneously between more than two particles). The Boltzmann equation provides information on the particle distribution in velocity and configuration space. (Details of two techniques which provide approximate solutions to this equation are contained in the Final Report No. R-3288 for Low-Altitude Satellite Interaction Problem Investigation Study (Ref. 1).) For this study, the collision model considered only classical hard sphere particles.

The Monte Carlo procedure was used exclusively during the present study, whereas the previous study evaluated both the Monte Carlo and a small Perturbation technique. The results from both approaches correlated well at the higher altitudes where conditions approach free molecular flow, and where a Perturbation technique is appropriate. As the altitude decreases below 150 kilometers, the effects of introducing a body into the free stream will increasingly exceed the ability of a Perturbation technique to predict these effects on free stream conditions. Thus, the small Perturbation technique is generally not a suitable method for analyzing the interaction problem throughout most of the transition region for finite-sized vehicles.

"Monte Carlo" is the technique of using a simulated situation and random numbers to generate solutions from which information for the real case is then deduced statistically. The Monte Carlo approach ranges from being a strictly mathematical technique for evaluating the complicated multi-dimensional Boltzmann collision integral to a complete simulation of a number of molecules, with randomness introduced only in the initial conditions. A modification of this latter approach is the one used in the present development. It consists of simultaneously following a large number of particles which yields, to some degree, a "direct simulation" of the processes taking place. Because there are finite limits on computer storage space, a modification to the direct simulation technique was developed by G. A. Bird (Refs. 2 and 3) wherein the real gas is simulated by several thousand "sample" particles populated into cells of the sample space considered. For collision calculations, all the particles in one cell are

used as a representation of the local distribution function from which collision pairs are chosen at random, but in proportion to their collision probability based on the real gas. This preceding discussion applies to a general program including three-dimensional cases. A specific computer program for the generalized two-dimensional, two-fluid program is described as follows.

A. THE GAS MODEL

The program conducts numerical experiments with a model binary gas. The real gas is simulated by several thousand rigid-sphere molecules which are considered to be a representative sample of the many billions of molecules in the corresponding real gas. The positions and velocity components of the simulated molecules are stored in the computer and typical collisions are computed among them as a time parameter is advanced. For a two-dimensional program, the flow is either z-independent or axi-symmetric, as shown in Figure 1a, so only two position coordinates need be stored for each simulated molecule, but three velocity components must be stored. (Z-independent means that the body dimension parallel to the z-axis and transverse to the free stream flow direction is very large, so that flow conditions will be similar in any plane perpendicular to this z direction.)

The computation of collisions starts at zero time with the molecules moving along the flow axis at the required free-stream Mach number. The body is inserted into this flow at zero time and the desired steady flow is obtained as the large-time solution of the resulting unsteady flow.

B. THE SAMPLE SPACE

The free-stream flow is in the positive x direction and the simulated region is bounded by the x-axis as a line of symmetry, and by the upstream, outer, and down-stream boundaries. These boundaries must be set sufficiently far from the body to eliminate interference. A suitable separation can be determined by varying the distance and observing the effects. The simulated region is divided into a number of cells which are sufficiently small for the change in flow properties across the cells to be small.

Typically, three levels of cell sizes may be specified. This permits the use of small cells in the regions where the gradients of the flow properties are large, while large cells will suffice where the gradients are small. The entire simulated region is covered by the first-level (largest size) cells. A region of these cells may be specified as the second-level cell region. A region of the second level cells may similarly be replaced by the third-level cell system. Figure 1b shows a typical cell geometry for flow about a body.
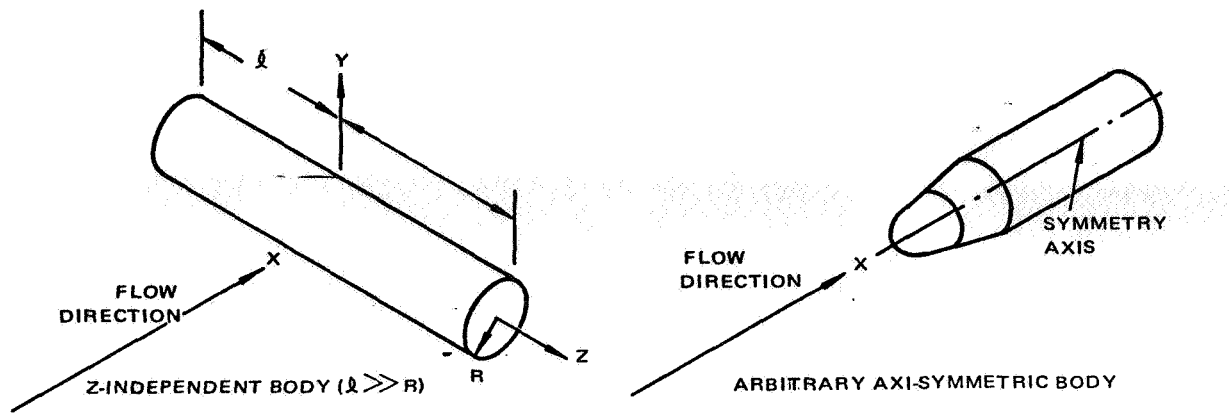
A. Pictorial Representations of Typical z-independent and Axi-Symmetric Bodies
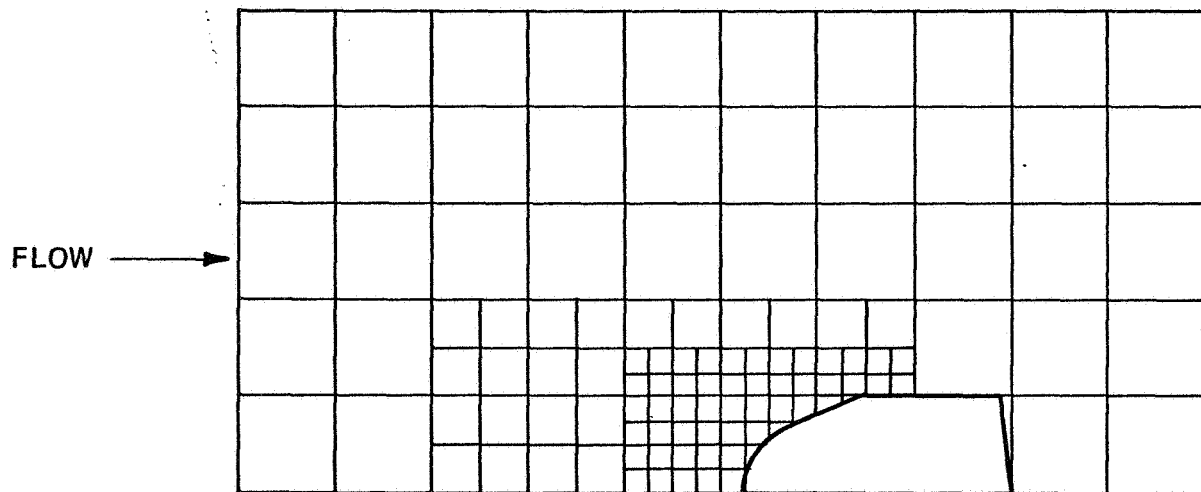
B. Cell Geometry for Arbitrary Body Showing Three Levels of Cell Size

Figure 1.   Pictorial Representation and Cell Geometry for
Axi-Symmetric and Arbitrary Bodies

C. THE FLOW CALCULATIONS

The first step is to generate the initial, or zero time, configuration of molecules. The molecules are distributed over the simulated region and the velocity components assigned are appropriate to a gas in Maxwellian equilibrium and moving at the required Mach number. The body is then inserted into the flow and the molecules are allowed to move and collide among themselves. The "move" and "collide" processes are uncoupled by computing collisions appropriate to a time interval Δt_m and then moving the molecules through distances appropriate to Δt_m and their instantaneous velocities. The distortion produced in the molecular paths by this approximation is small as long as Δt_m is small compared with the mean time between collisions.

The distribution of the molecules in the z-independent geometry is simple: uniformly random in both directions normal to the z-axis (x and y), and the cell quantities are in terms of cross-sectional areas. In axi-symmetric geometry, however, the cell quantities must be considered in terms of annular volumes. In this case, the cells are much smaller near the flow axis than away from it. A different procedure must be used to obtain sufficiently large statistical samples of flow properties in a reasonable amount of computer running time.

The procedure adopted is to assign a weighting factor to each molecule such that a simulated molecule far from the axis represents a larger number of real molecules than a simulated molecule near the axis. The weighting factors are applied at boundaries between cell layers. In the cylindrical region containing the flow axis, the molecules have a weighting factor of unity. Different integer weighting factors are applied in up to five annular regions. The value in any region n is determined by:

$$(WF)_n = \frac{r_n + r_{n+1}}{(WF)_1 \times (WF)_2 \times \ldots \times (WF)_{n-1}} = \frac{r_n + r_{n+1}}{\displaystyle\prod_{k=1}^{n-1} (WF)_k}$$

where

$(WF)_k$ is the kth weighting factor,

r_{n+1} is the upper boundary (expressed in number of cells) of the annular region, and

r_n is the lower boundary of the region.

II-4

Since the change in flow properties over the width of each cell is small, the molecules in a cell at any instant may be regarded as a sample of the molecules at the location of the cell. The relative location of the various molecules within the cell can then be disregarded. A pair of molecules is chosen at random from those within the cell under consideration and is retained or rejected in such a way that the probability of retention is proportional to the relative velocity. When a pair is retained, a typical collision is computed between the two molecules and the new velocity components are stored in place of the old ones. For hard sphere collisions, all directions for the new relative velocity vector are equally probable.

In general, the relative number ratio of the two types of molecules in the binary gas will differ from unity, requiring the computation of four different types of collisions: A-A, A-B, B-A, B-B. There is, therefore, one time counter for each type of collision in each cell. For each collision, the correct time counter is advanced for the cell by an amount appropriate to the collision parameters. The probability of collision, and therefore the time advancement per collision, is made proportional to the number of molecules in the cell, and the relative velocity and collision cross-sections of the colliding molecules. Collisions are computed in each cell until all the time counters have advanced through Δt_m. When this procedure has been carried out for all cells, the overall experiment time is advanced by Δt_m and the molecules are moved through appropriate distances.

The set of molecules in each cell changes as the molecules are moved and appropriate conditions must be applied at the boundaries of the region being simulated. The upstream boundary normal to the free-stream direction is treated as a source of molecules with velocity components representative of molecules moving in equilibrium at the free-stream Mach number. Any molecule which moves back upstream across this boundary is regarded as being lost and is removed from the sample. The plane of symmetry along the x-axis is regarded as a specularly reflecting surface in the z-independent geometry, but has no special significance in the axi-symmetric geometry. The outer and rear surfaces present additional complications. The procedure that has been developed introduces only a small reflected disturbance. A molecule is regarded as lost if it moves outward across the boundary. A molecule that moves inward from the boundary during the time interval Δt_m through a distance greater than its original distance from the boundary, causes a new molecule to be added to the sample via a parallel trajectory from outside the experiment region.

Interactions with the body are also computed. The body consists of a number (up to eight) of conic sections. Each section must be separately specified according to the coefficients of the defining equation:

$$ax^2 + by^2 + cz^2 + 2fyz + 2gxz + 2hxy + 2px + 2qy + 2rz + d = 0$$

A major restriction for the two-dimensional program is that the body must be either a surface of revolution (quadric) about the flow axis (x-axis), or an airfoil surface which has the following geometry: chord-line coincident with the flow axis, and span along z-axis (z-independent geometry). The surface generated will be at zero angle-of-attack, and the lower surface will be a mirror image of the upper surface.

For the purpose of computing the momentum and energy transfers to the surface, each region of the body can be subdivided into smaller sections. Within these smaller sections, the following three parameters must be specified: wall temperature/gas temperature, energy accommodation coefficient, and tangential (momentum) accommodation coefficient.

After the flow has settled down to a steady state, the number flux, momentum, and energy transfers to the surface are accumulated and used to compute the aerodynamic data. The time required to establish steady flow is usually assumed to be close to the time required for the free-stream flow to traverse several body lengths. The overall number flux, drag, and heat transfer coefficients are determined, with their distribution along the surface.

Flow field properties are also computed. Instantaneous values are sampled at appropriate time intervals and these are time-averaged for greater accuracy. The time interval for sampling is assumed to be on the order of the time for the free-stream flow to traverse one cell. Number density, flow velocity, and temperature are printed at each cell location. As an indication of the degree of non-equilibrium, the temperatures based on the individual velocity components are also printed.

The program is written in FORTRAN IV and has been made operational* (debugged) on the GSFC IBM 360-75 and 360-91 computers. The program is also compatible with the ITT IBM 360-65 computer. The -91 running time is several times faster than either the -65 or -75.

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* It should be noted that under certain initial conditions the 360-91 computer will hang up early in the program as a result of a small infinite loop. The cause for this loop was not determined during the period of performance of this study; however, it probably lies in the method of random number generation or in the technique for specifying dimensions (the dimensions and positions generally cannot be specified exactly and the method of rounding-off numbers may cause looping). A minor modification to the input data enables the program to run properly. The differences are very small between the program results at the time of stoppage and those at a similar time when the program runs to completion, which provides us a high degree of confidence in the general technique and results. Also, the results produced on the -75 and -91 are not always exactly the same for the identical program; however, differences are within statistical limits.

SECTION III

DISCUSSION OF RESULTS

A.   THE GENERALIZED TWO-DIMENSIONAL, TWO-FLUID PROGRAM

One of the most important results of this entire study was the generation and documentation of a generalized two-dimensional, two-fluid program. The main purpose for this effort was the limited applicability and inflexibility of the original programs. Since these programs were adapted from existing material for the purpose of obtaining preliminary technical results, many computational routines or procedures were illogically fragmented throughout them. Furthermore, separate but basically similar programs existed for each different geometry. The programs were awkward and inefficient in terms of storage requirements, computational time, and the time required to make program changes. The work effort to reorganize, generalize, and otherwise improve the programs was divided into several subtasks, the results of which are described in the following paragraphs.

The first revision was a rearrangement of the computation activity to make the sphere program more logical and reduce the storage requirements. Concurrent with the reordering, the program was separated into sub-programs, either functions or subroutines. It was now possible to alter a specific sub-program without interfering with or modifying the remaining sub-programs.

The second revision was to incorporate the unique features of the transverse cylinder program into the sphere program so that either type of geometry, z-independent or axi-symmetric, could be run with just one program.

The third revision was to modify some of the sub-programs and create those new sub-programs necessary to use a generalized body geometry concept.

The important sub-programs are described in the following paragraphs.

1.   Subroutine GAS

This sub-program generates the position coordinate and velocity values of the initial distribution of particles. Also, it computes the populations and densities in all the cells. Initial position distribution (radial for axi-symmetric geometry) and velocity distribution (Maxwellian, plus supersonic flow speed along the axis) can be changed easily by changing the corresponding instructions.

2.   Subroutine COLIDE

This sub-program randomly selects colliding particle pairs in each cell and advances the cell's elapsed experiment time by an amount appropriate for that collision. The current collision mechanism is purely elastic between hard sphere particles, but can be easily modified. This is the first sub-program in the major program loop.

3.   Subroutine MOVE

This sub-program translates each particle the distance appropriate to its velocity and the fractional collision time (Δt_m). If a particle-body surface collision occurs, the trajectory segment after collision is determined by the velocity of reflection and the amount of fractional collision time left.

4.   Subroutine INTERS

This sub-program determines if a particle trajectory segment actually intersects the body surface. This subroutine is called by subroutine MOVE for only those trajectory segments in the vicinity of the body surface. If the trajectory segment actually does intersect the body surface, the coordinates of the collision point on the body surface are determined, and then this subroutine calls subroutine DRAG.

5.   Subroutine DRAG

This sub-program computes the particle velocity of reflection according to the mode selected by the user, i.e., a combination of specular and diffuse reflections, with the energy accomodation coefficient specified for the diffusely colliding particles. Also, if steady state conditions have been reached by the experiment, momentum and energy quantities are accumulated, e.g., skin friction, pressure, and heat transfer.

6.   Subroutine FLOW

This sub-program adds the appropriate number of new particles to the experiment through the up-stream boundary. In doing so, the subroutine assigns the correct velocity components (Maxwellian plus hypersonic flow speed) and position coordinates (radial for axi-symmetric geometry) to the particles.

7. Subroutines ACCUM and AVRGE

The first subroutine computes the temperatures, densities, and average particle velocities in each cell at a specified periodic interval. The latter subroutine uses these averages to compute time-averaged temperatures, densities, and particle velocities.

8. Subroutines PRINT1 and PRINT2

The first subroutine prints out the body surface flow data after the experiment has reached steady state conditions. The second subroutine prints out flow field information, starting with a printout at zero time of the initial flow field configuration. These sub-programs are the last ones in the major loop.

In addition to these major sub-programs, there are several others that perform essential tasks in the program. They include RAND (random number generator) HEIGHT (body height at given x coordinate), CELL-ZERO-SBTRCT (cell volume calculating system), and SIMPSN-FNCTN (body surface area calculating system).

A major product of this study is the complete documentation for the generalized two-dimensional, two-fluid program (Ref. 4), which has been provided to Goddard Space Flight Center (GSFC) under separate cover.

The rationale for extending the program to generalized body geometry is as follows. In the free molecular flow regime, the local fluxes to the spacecraft body are essentially determined by the local geometry alone. In the transition region, the shape of the entire body will influence the local flux so that it is important to consider shapes other than the idealized sphere and long cylinder. In addition, even though this study considered only z-independent and axi-symmetric bodies with respect to the flow direction, the generalization to shapes other than a sphere and a long cylinder permits the program to be more representative of real physical cases.

The manner in which the body geometry is introduced into the computation has been already described in Section II, Theoretical Foundation. In essence, the computer solves the problem of the intersection of a straight line with a quadric surface. The general second degree equation is modified to represent specific conic sections of interest by assigning values to the appropriate coefficients in the equation. For axi-symmetric geometry, the conics are then rotated about an axis of symmetry to generate the quadric surface. Thus, the program contains the most general quadratic equation which can then represent any desired conic section by simply programming appropriate values for the coefficients.

An important check was successfully made to verify that the program would correctly handle multiple body collisions by one particle in a single time increment. This case could occur with a concave body shape. The geometry used for the test was a small sphere partly buried in a larger sphere as shown in the sketch below.

FLOW
DIRECTION
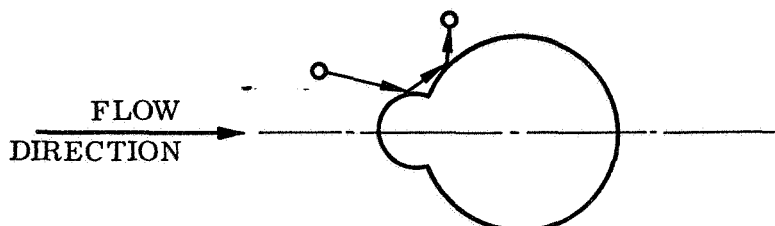
The reflection boundary conditions subroutine was also generalized. The boundary conditions can now be changed by changing certain cards in the DRAG subroutine. Presently, the reflected particles are considered to consist of two types, specular and diffuse. The fraction, σ, is scattered diffusely and $1-\sigma$ is scattered specularly, where σ is the tangential momentum accommodation coefficient. The diffuse component will have Maxwellain velocity distributions based on a temperature which is related to the body temperature through a specified energy accommodation coefficient. More sophisticated models for the reflection procedure can be easily incorporated, provided their form can be specified by a function giving the probability of transition from incident to reflected velocities. At present such transition probability information is not available; therefore, no attempt was made to program such a procedure in this study.

The sensitivity of the surface flux data to the proximity of the sample space boundaries was examined. Several test runs were made keeping all parameters constant except the separation distance from the body to the upstream and transverse or side boundaries. (A previous investigation showed that at high Mach numbers the flow conditions near the body surface were insensitive to the distance to the downstream boundary for all distances greater than one body diameter.) The transverse boundary location has no apparent effect on the surface flux conditions provided the distance from the body surface to the transverse boundary is greater than the distance from the body to the upstream boundary divided by the Mach number, S. This can be expressed mathematically as

$$\frac{(S)(Y)}{X} > 1$$

where X and Y are the distances from the body surface to the upstream and transverse boundaries, respectively.

At high Knudsen numbers, Kn, the flow field conditions near the surface are sensitive to location of the upstream boundary. It was found that for such high Kn, X must be sufficiently large so that the solid angle subtended by the body to any point on the upstream boundary is small (0.0314 steradians or less). At lower Kn (but greater than Kn = 0.3), it was found that as long as X was at least 3 mean-free-paths (m.f.p.), there was no measurable effect with increasing X. The upstream boundary location was chosen by first considering the solid angle requirement. If this resulted in X > 3 m.f.p., the location of the upstream boundary was made equal to approximately 3 m.f.p.

In order to both test the operational aspects of the program on some reasonably realistic "production runs", and to gain insight into some of the physical phenomena and their orders of magnitude, eleven "production runs" were computed. All of these runs were for a spherical body in order to supplement the rather limited data obtained for this geometry under Contract No. NAS5-11016 (Ref. 1). For five of the runs the Knudsen numbers ranged from 0.3 to 30.0, the mass ratio was fixed at 7, and the light mole fraction was 5 percent (simulating a trace of helium in a nitrogen-oxygen composite primary constituent). In the remaining six runs, the mass ratio was 1.8 (simulating atomic oxygen in a molecular nitrogen-oxygen composite), while the light gas mole fraction varied from about 5 to 50 percent, and the Knudsen numbers were one and three. The other important physical parameters such as Mach number (S), ratio of body temperature to that in the free stream (TR), and molecular diameter ratio (DIR) of the two species, were all chosen to correspond to physically realistic values. The parameters were evaluated based on satellite velocities, atmospheric temperatures from COSPAR 1965 Tables, (Ref. 5), approximately 300°K vehicle, and equivalent hard sphere collision cross-sections based on energy arising from vehicle velocity. The tangential and energy accommodation coefficients were taken to be unity in the absence of specific information on realistic values. Table 1 presents a tabulation of the major physical parameters for the eleven "production" runs.

Some typical results from the runs listed in Table 1 and, in some cases, comparison to the results for long cylinders transverse to the flow from Reference 1 are presented in Figures 2 through 5.

The main emphasis is to indicate the kinds of phenomena that arise and to present the qualitative features of these effects on data reduction. Figure 2a shows some mass density contours referenced to the free-stream value for a Mach number S = 15 flow around a sphere at a Knudsen number Kn = 30. Figure 2b gives the same information for an S = 25, Kn = 1 flow. In both cases there is a large increase in density in the vicinity of the stagnation point. At the lower Knudsen number, where inter-particle collisions are important, the density rise is much steeper and the density levels higher. Very near the stagnation

TABLE 1. MAJOR PARAMETERS FOR PRODUCTION RUNS

Run	Kn	S	N_B/N_A	M_B/M_A	TR	DIR
1	0.3	27	20	7	1.5	1.7
2	1	25	20	7	1.2	1.7
3	3	23	20	7	1.0	1.7
4	10	19	20	7	0.75	1.7
5	30	15	20	7	0.50	1.7
6	1	25	20	1.8	1.2	1.34
7	1	25	3	1.8	1.2	1.34
8	1	25	10	1.8	1.2	1.34
9	3	23	10	1.8	1.0	1.34
10	3	23	3	1.8	1.0	1.34
11	3	23	1	1.8	1.0	1.34

Kn	is	Knudsen number
S	is	Mach number
N_B/N_A	is	Free-stream number density ratio of the two species
M_B/M_A	is	Free-stream mass ratio of the two species
TR	is	Temperature of the vehicle ratioed to the free-stream temperature
DIR	is	Ratio of molecular diameters of the two species

point the density exceeds 60 times the free-stream value while in nearly free-molecular flow (Kn = 30) the corresponding value is only around 20. The resolution of the computation does not enable predicting the precise value at the stagnation point, but the results certainly appear to show a trend compatible with theory. Free molecular theory predicts a stagnation point density ratio

$$\frac{\rho_S}{\rho_\infty} = \frac{1}{2}\left[1 + \sqrt{\frac{10\pi}{3}}\, S\right]$$
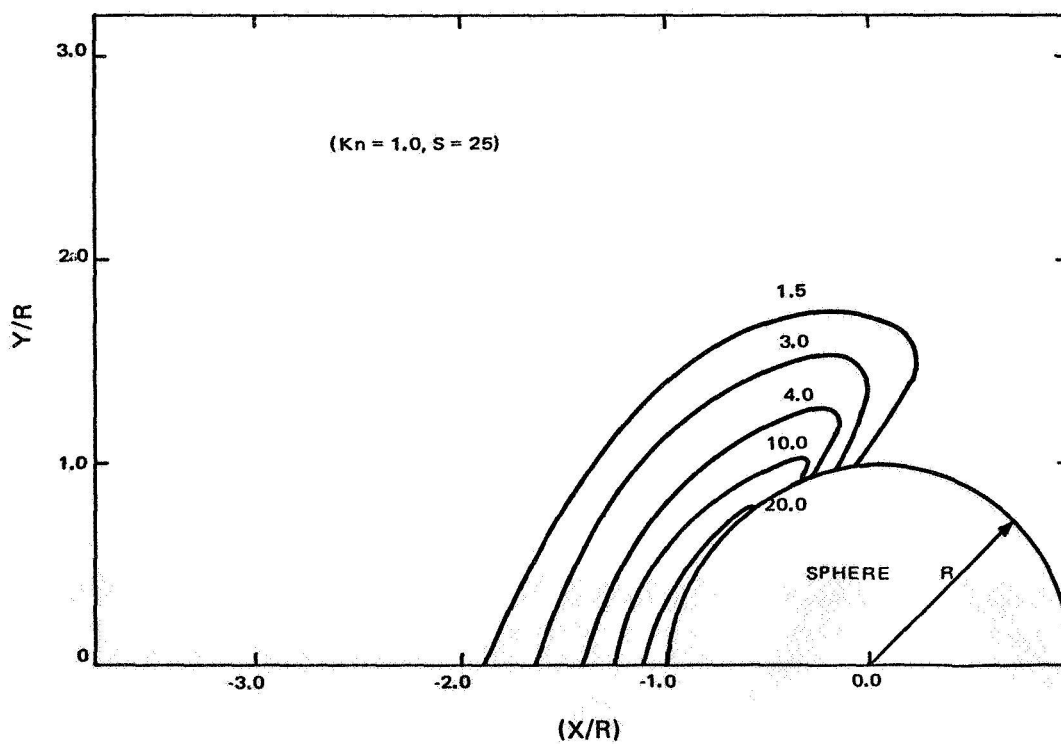
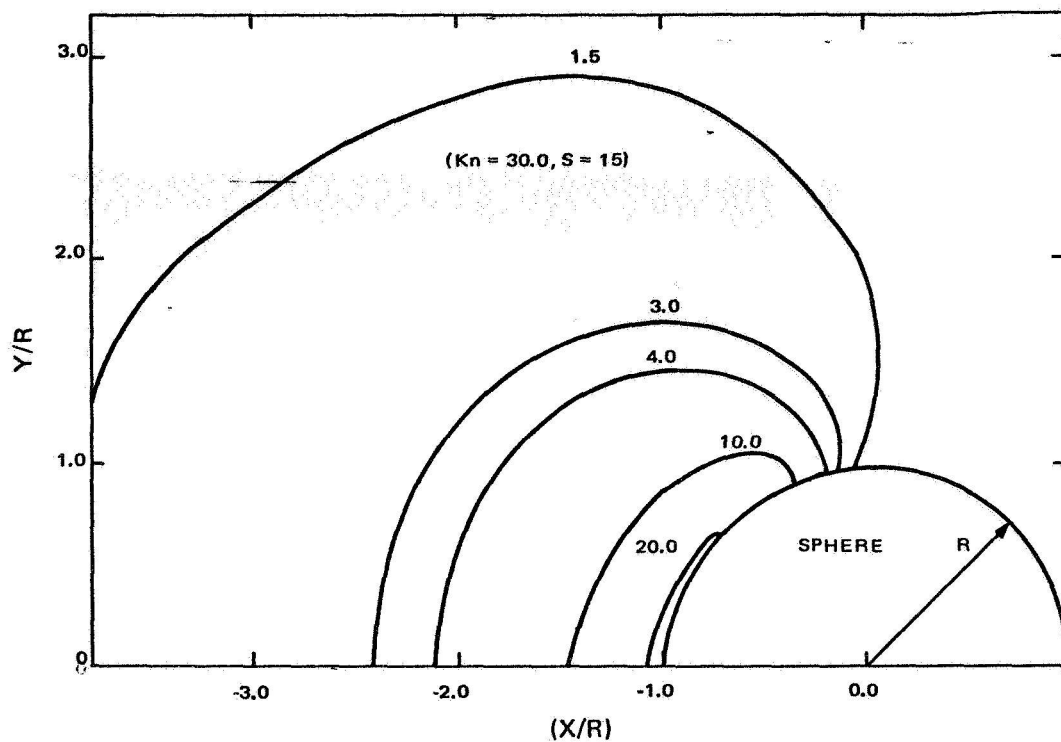which in the Kn = 30 run would be 24.3.

Figure 2. Density Contours for Flow About a Sphere; Perfect Accommodation is Assumed at a Body Temperature Equal to the Free-Stream Gas Temperature. (All Density Levels are Referenced to the Free-Stream Values)
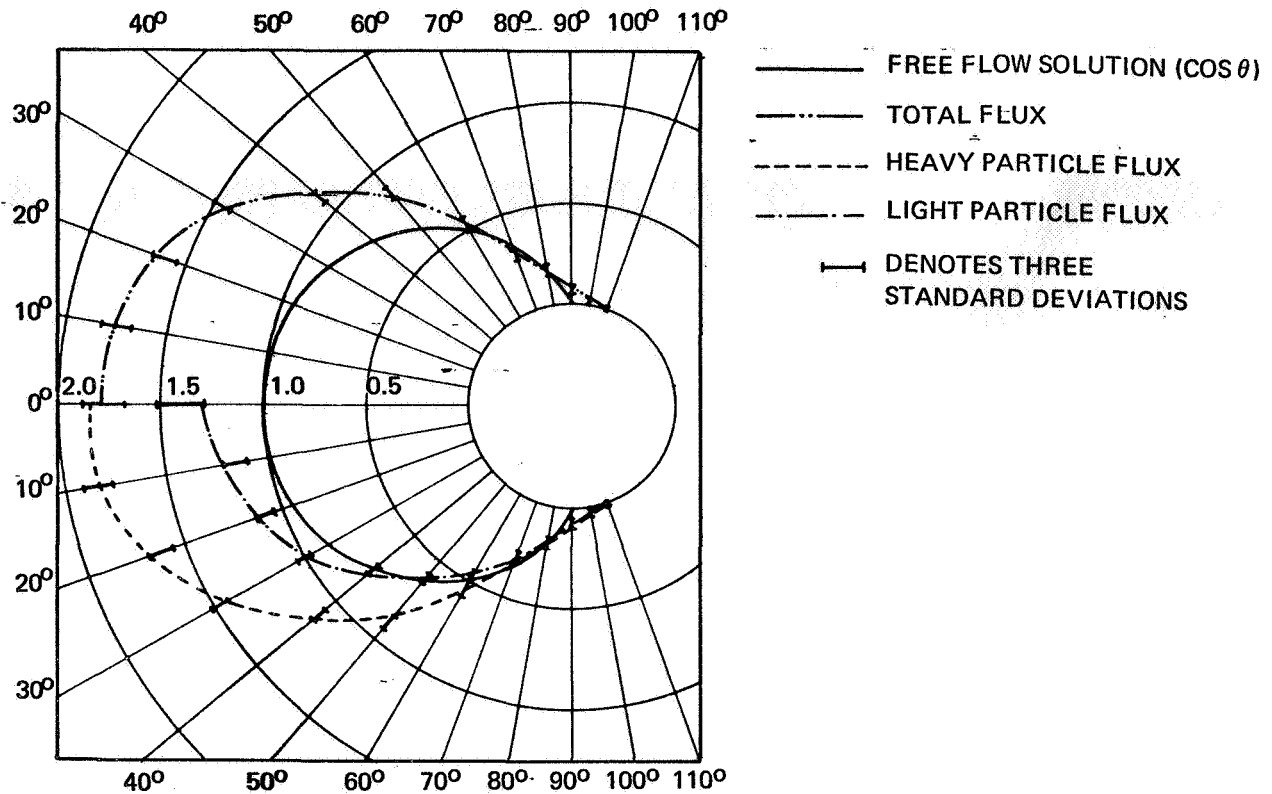
Figure 3. Angular Distribution of Particle Fluxes Per Unit Area on a Sphere. (S = 25, Kn = 1. 0, Perfect Accommodation, Mass Ratio of 7.) Numbers shown are Referenced to Free-Stream

Continuum theory (Kn → 0) predicts $\rho_s/\rho_\infty \approx 1.47S^2/TR$ which for S = 25 and TR = 1. 2, corresponding to the Kn = 1 run, would give $\rho_s/\rho_\infty \approx 275$, well in excess of the results at Kn = 1. The main reason for presenting the information in Figure 2 is to show that particles arriving at the body from the free stream have to transverse a region of very high density even at Knudsen numbers around unity and therefore the probability of free stream particles arriving at the surface without collision with other particles near the body is reduced below that which would be estimated on the basis of the free stream mean-free-path.

Figure 3 gives the angular distribution of particle number fluxes per unit area for the same flow conditions as described in Figure 2b. The solid curve represents the flux that would exist under free molecular conditions (cosine law for this high speed ratio). The upper dashed curve represents the total number flux per unit area relative to the free-stream value. Note that over virtually the entire forward portion of the sphere this flux is well above the free-molecular value, with nearly a factor of two increase at the stagnation point. The lower two dashed curves show the fluxes of the heavy and light species, each referenced to its free-stream value. Although both species' fluxes are in excess of the free molecular result, the heavy gas is over-abundant near the
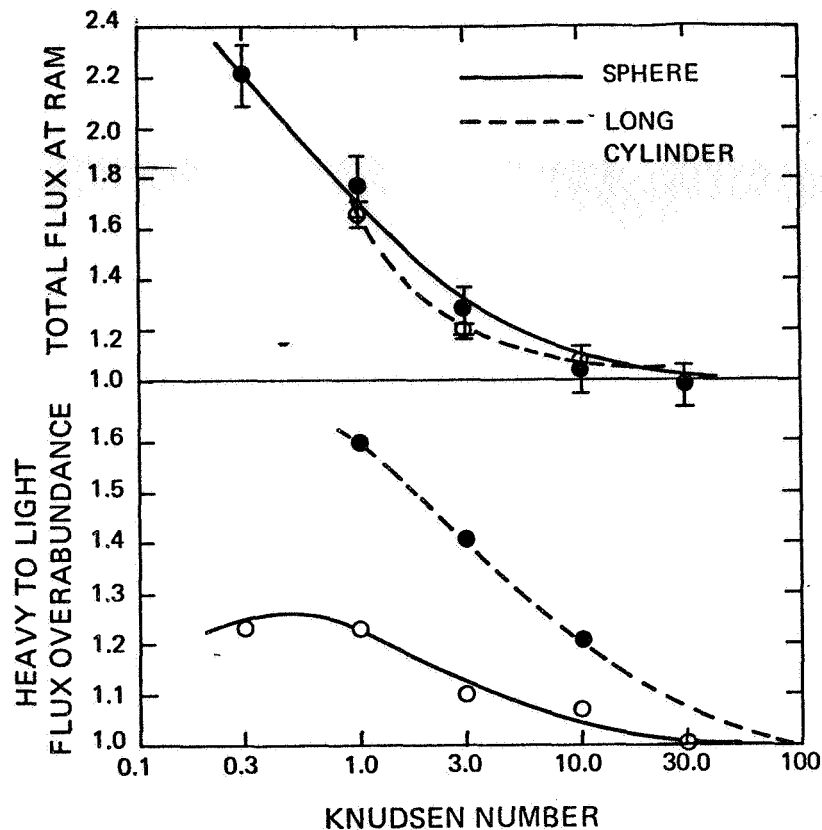
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Figure 4. Variation of Flux at the Stagnation Point with Knudsen
Number (Mass Ratio for Gas is 7 for Sphere Case and
10 for Cylinder)

stagnation point. A reduction of sensor data to obtain relative concentrations
without inclusion of the interaction effect would underestimate the light species
mole fraction by approximately 30 percent. Note that although Figure 3 shows
the results for a 5-percent mole fraction of lights, the results would be very
nearly correct for any smaller fraction (trace situation). The trace situation
causes particular computational difficulties because of the small sample size.
Most difficulties are circumvented in the program by having an equal sample of
each specie, where the sample trace particles represent fewer real ones (this
procedure is explained in the program documentation). However, since only a
small fraction of cross collisions is taken into account in their effects on the
major constituent, the statistics for this effect are still very poor in the trace
situation. As the trace concentration becomes small the effect of cross-colli-
sions on the major constituent, as well as the ratio of self-collisions to cross-
collisions for the trace gas, is proportional to the trace mole fraction and thus
becomes negligible. The results for both species can therefore be obtained
from the 5-percent mole fraction results by scaling directly on the free-stream
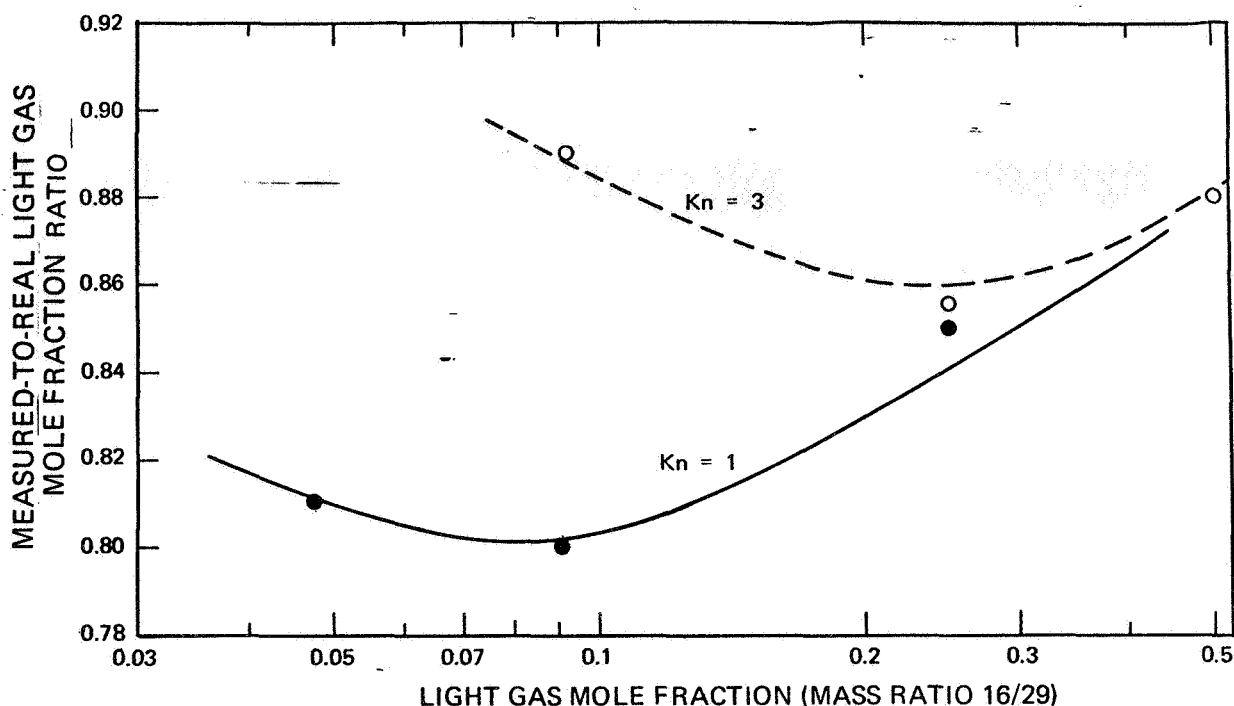densities, with an inherent error of about 5 percent.

Figure 5.   Variation of Ratio of Measured Light Particle Mole
Fraction to that in Free Stream at the Stagnation
Point on a Sphere with the Actual Free-Stream Mole
Fraction. (Mass Ratio is 1.8, S = 25)

Figure 4 gives an indication of the variation of stagnation point (ram conditions)
fluxes with Knudsen number or equivalently, altitude. (For a one-meter body,
Kn = 0.3 corresponds to approximately 100-km altitude, and Kn = 30 to about
140 kilometers.) Note the large increase in total flux at the stagnation point
with decreasing altitude in Figure 4. Neglect of this effect would result in
gross over-estimation of the ambient atmospheric density levels in this altitude
regime. The dashed curve for a long cylinder transverse to the flow (Ref. 1)
is shown for comparison purposes. Although perturbation theory predicts
greater departures from free molecular results for the cylinder than for the
sphere at high Knudsen number, apparently by the time the Knudsen number is
down to about 10 these differences are not significant. Figure 4 shows the heavy-
to-light flux ratio at the stagnation point referenced to the free stream for the
sphere from the present runs, and for the long cylinder from Reference 1. The
sphere results are for a 5-percent mole fraction of light gas and a mass ratio
of seven, while the cylinder results are for a 50-percent mole fraction and a
mass ratio of 10. Both the increase of the transverse body dimension (in the
long cylinder), and the increase of the mass ratio tend to increase the heavy
particle over-abundance. The previous results for the cylinder, as well as the
results in Figure 5, tend to indicate that the effect of mole fraction is not too
pronounced on the relative abundance increase over the free-stream value.

Figure 5 shows the variation of the light-to-heavy particle flux ratio referenced to the free stream at the stagnation point for flow about a sphere at a mass ratio of 1.8 (29/16) and Knudsen numbers of Kn = 1 and Kn = 3, as a function of the free-stream mole fraction of the light gas. Although the information is not very extensive, the main trends are quite clear. On this figure both free-molecular and continuum results would be unity independently of mole fraction. For every mole fraction there must, therefore, be a knudsen number where the deviation from unity is maximum. From the present results it appears that for the mole fractions shown, this maximum deviation occurs at Knudsen numbers less than one. The variation with mole fraction for a specific Knudsen number does not appear to be monotonic, although the variation in the current results is too small to permit any definite conclusion pending additional runs to establish definite trends. One effect is, however, clearly apparent; even at this moderate mass ratio, the inferred mole fraction of the light species could be 20 percent too low if the interaction is not incorporated into the data reduction procedure.

Although the results presented above are only indicative of the kinds of phenomena that effect data interpretation in the 90- to 150-km altitude range, they are sufficient to show that accurate data can only be obtained by including the interaction effects in this altitude regime.

B.   THE INTERNAL FLOW PROGRAM

The results presented in the previous section are indicative of some of the kinds and expected orders of magnitude of phenomena that will arise in the interpretation of aeronomic data in the transition region. It is also very important to understand the effects of the altered distribution function of the particles entering a measuring instrument on the internal behavior of such an instrument. An analogous Monte Carlo program for internal flow was developed to provide information of this nature for data reduction.

The geometry constraints of the cavity are similar to the external flow program (axi-symmetric case); that is, a finite number of connected quadric sections with a common axis of symmetry. In this program, however, the symmetry axis is not restricted to alignment with the flow direction—the entrance to the cavity can be at any arbitrary angle to the flow. The axis of symmetry and the flow direction define a plane of symmetry (the x-y plane), with the body-flow properties mirror images on opposite sides of the plane (see Figure 6). The particle velocity components are obtained by adding the randomly generated, thermal velocities in the three coordinate directions to the corresponding flow velocity components. The thermal velocities are generated the same way as in the external flow program. Also, the total velocity components are fitted to the same type of velocity distributions.
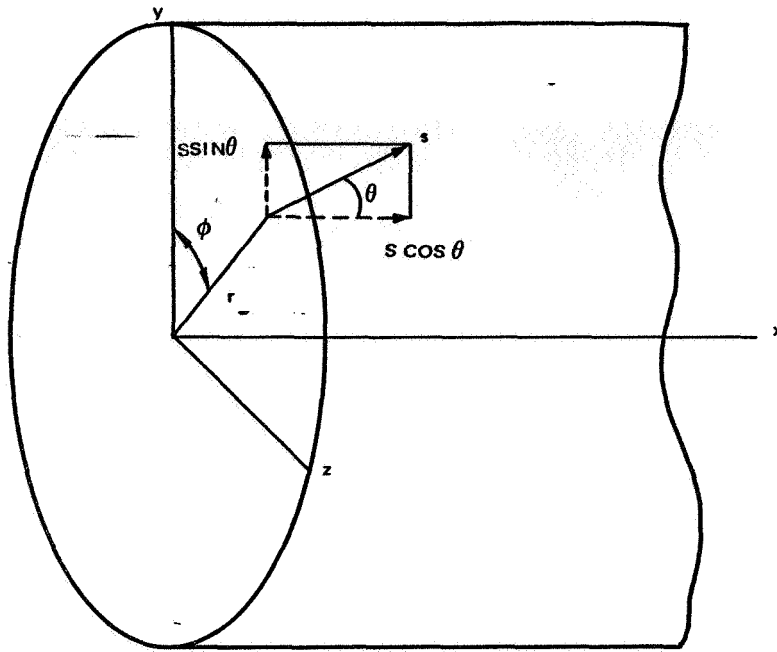
Figure 6. Entrance Region of Internal Flow Program (Particle is
Located at x = 0, y = r cos ϕ, z = r sin ϕ; Flow
Velocity is v_x = S cos θ, v_y = S sin θ, v_z = 0)

There must be three position coordinates for each particle. The initial positions
are generated as follows. The x value is set to zero. A radial component is
generated the same way as the radial component in the external flow axi-sym-
metric case. An azimuthal angle (ϕ) between zero and pi is randomly gener-
ated (see Figure 6). The y and z coordinates are then generated from the
radial and azimuthal values.

Using these x-y-z values and the velocities, the particle is translated into the
entrance region from the x = 0 plane by a random part of $v\Delta t_m$. The resulting
position values are used as the initial values for that particle. If a collision
with the wall occurs, it is handled the way collisions are normally handled.
Thus, the internal flow program is three dimensional.

The geometry investigated in this study consisted of an entrance region followed
by a cavity describable by not more than eight connected quadrics. The limiting
number eight is based on practical convenience and allocated storage; it does not
indicate a fundamental program limitation.

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The distribution function of the particles entering the internal region can be specified by a wide range of analytical formulae. Currently, only local Maxwellian distributions around a mean-flow velocity at an arbitrary angle with the cavity axis have been considered. As more information on the actual distributions at the body surface becomes available from the external flow program, the representation of the distribution function can be improved upon. The procedure by which particles are introduced into the region of interest is also similar to that of the two-dimensional external flow program except that no particles can enter from the side or back boundaries.

It is appropriate here to briefly discuss the three-dimensional, two-fluid external flow program. The processes described above for computing off-axis flow for the internal flow program also apply to the three-dimensional external flow program. The major difference is that particles can also enter and leave through the side and downstream boundaries in the external flow program. A unique probability distribution of "entering" particles is being developed which will generate appropriate velocities and positions for any location on the sample space boundary. The upstream boundary procedures for determining initial particle velocities and positions are the same in both programs. ("Upstream boundary" as used here refers to the sample space boundary in front of the body and normal to the body axis of symmetry.)

For cavity entrance regions with an opening D much smaller than the cavity size, the time to reach steady-state conditions is very long if the initial population within the cavity is not chosen to be consistent with the entrance flux. To circumvent extremely long computer running times the proper relation between the cavity population and incoming flux is generated from the input and output transmission coefficients of the entrance region. These transmission coefficients are computed by considering only the trajectories and wall collisions of particles in this region. Particles within the cavity are considered to be in thermal equilibrium and any particles that are reemitted will have a Maxwellian velocity distribution. The need to perform trajectory and collision computations within the cavity is thereby eliminated.

The accommodation coefficients and temperatures can be separately specified for each different cavity segment. Computations of particle-particle and particle-wall collisions, particle trajectories, and averaging procedures are similar to those of the external flow program.

The internal flow program was examined for two geometries. The first case was for a very short entrance tube, $L/D = 1/10$ (simulating an orifice). The second case was for $L/D = 1$, where L is the length of the entrance tube and D is the entrance diameter. In both cases, the size of the cavity is very much greater than the entrance diameter, D.

The results of case 1 (L/D = 1/10) matched analytical results for an orifice (L → 0) opening into a cavity whose size approaches infinity.

Case two was examined for a variety of incidence angles (θ) and Mach numbers (S). The results agreed with published numerical solutions (Ref. 6), for low and high Mach numbers (S = 1, 20) and at all incidence angles which were examined (θ = 0°, 30°, 90°). At S = 5 and θ = 30°, 90°, the difference between the program and referenced results were well beyond several standard deviations. The numerical technique used in Reference 6 is particularly subject to error in the range of moderate Mach numbers; therefore, the investigators feel a greater degree of confidence in the results obtained in this study over those contained in Reference 6, although only more detailed comparisons could be conclusive.

Figure 7 shows the computed ratio of pressure inside a large cavity with an entrance L/D = 1, to the pressure in an infinite cavity behind an orifice (L/D → 0), as a function of incidence angle and Mach number.

C. SIMULATION OF TWO OR MORE GASES BY A SINGLE COMPOSITE GAS AND TRACE GAS OPTIMIZATION

All computers currently in service have practical limits in terms of storage capacity and operational running time for any given program. The first restriction can be partially circumvented by limiting the number of data samples and improving the program efficiency, but there are practical limits to these techniques. Furthermore, any reduction in sample size must be offset by longer computer running time to acquire reasonable statistical results. Competition by other programs and operating costs limit the computer time available to any single program.

A two-specie gas can be readily accommodated in the two- and three-dimensional programs which were investigated in this study using the IBM 360-75 and -91 computers. The histories of several thousand particles could be followed sufficiently long to achieve meaningful results in reasonable computer running time (approximately 20 minutes on the IBM 360-91). Furthermore, this sample size was adequate to sufficiently populate each cell so that the interaction results are representative of the true gas. However, in the three-dimensional case (including flow not aligned with the symmetry axis), the two-fluid program approaches the storage limit of the IBM 360-91 and -95 computers. (The three-dimensional, two-fluid program requires approximately 900k bytes and will run about 40 minutes for the same size problem as typical ones run during this study. The IBM 360-91 has an active storage of approximately 1200 kbytes; the 360-95 has an active storage of approximately 4400 kbytes.)
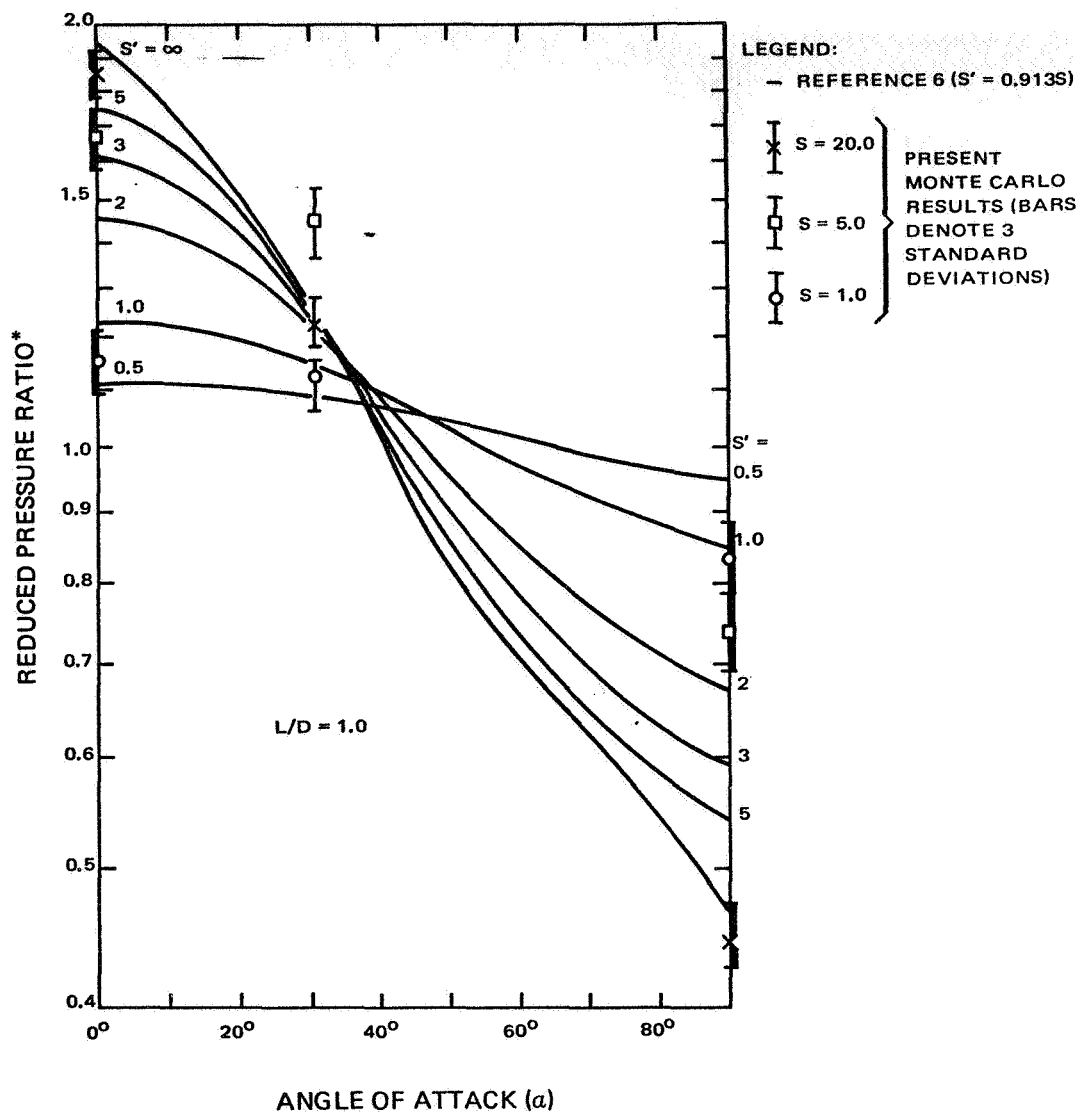
*REDUCED PRESSURE RATIO = PRESSURE IN A CAVITY BEHIND AN ENTRANCE TUBE OF LENGTH TO DIAMETER RATIO OF L/D, REFERENCED TO THE PRESSURE IN A LARGE STAGNANT RESERVOIR BEHIND AN ORIFICE (L/D → 0).

Figure 7.   Ratios of Pressure Inside a Large Cavity with Entrance L/D = 1 to Pressure in Large Stagnant Reservoir Behind Orifice (L/D → 0); Comparison of Computed-to-Published Results Obtained Numerically

If the same individual particle population sizes are retained, the introduction of a third specie will considerably increase the particle information storage requirements (50 percent). Furthermore, there are now nine collision possibilities which must be calculated, as opposed to four possibilities for the two-gas case. The compute-time required to calculate particle-particle collisions thus increases by a factor of 2.25, due to this effect, plus an additional 50-percent increase due to the larger number of particle trajectories to be followed.

The region of atmospheric interest does not consist of only a two-gas mixture. For example, at 110 kilometers, the approximate relative number densities of the four major components are:

$$(N_2) \approx 162$$

$$(O_2) \approx 35$$

$$(O) \approx 20$$

$$(A) \approx 2 \text{ (trace gas)}$$

Accordingly, for a computer analysis of the real physical situation, it will be necessary to devise some means of simulating the effects of two or more different gases by a single composite or synthetic gas.

One such technique was briefly examined in this study. The procedure is as follows: Using the 110-km atmospheric data, a first composite gas composed of N_2 and O_2 was calculated to have a new mass of 28.8 AMU. Assuming the molecular diameter is proportional to the square root of its mass, the ratio of the ($N_2 + O_2$) composite diameter to the 0 diameter is

$$\sqrt{28.8} \; : \; \sqrt{16} \; = \; 1.34 : 1,$$

and the mass ratio is 1.8 : 1.

At 110 kilometers, a 1-meter body traveling at a velocity of approximately 8.5 km/sec yields a Knudsen number very close to 1.0. Thus, the input data for the first case was:

Body Geometry	Sphere
Number Density Ratio N_B/N_A	197:20 $\cong$ 10:1
Mass Ratio M_B/M_A	28.8:16 $\cong$ 1.8:1
Molecular Diameter Ratio	1.34:1
Mach Number	25
Knudsen Number	1.0

where B refers to the $N_2 + O_2$ composite gas and A refers to 0. Mean body quantities were computed for this two-gas mixture and the results are shown in Figure 8.

Next, the mixture was considered to be a single gas composed of $N_2 + O_2 + 0$, having a new mass of 27.6 AMU. The total fluxes to the body surface were then computed based on this single gas for a Knudsen number again equal to 1.0. These results are also shown in Figure 8. Comparing the results of the two cases, it can be concluded that this simple simulation technique was successful in approximating two or more-major constituents by a single specie. The technique will be useful in studying trace gas effects. More complicated effects, such as atomic oxygen recombination on the body surface and other chemical interactions, were not considered in this study.
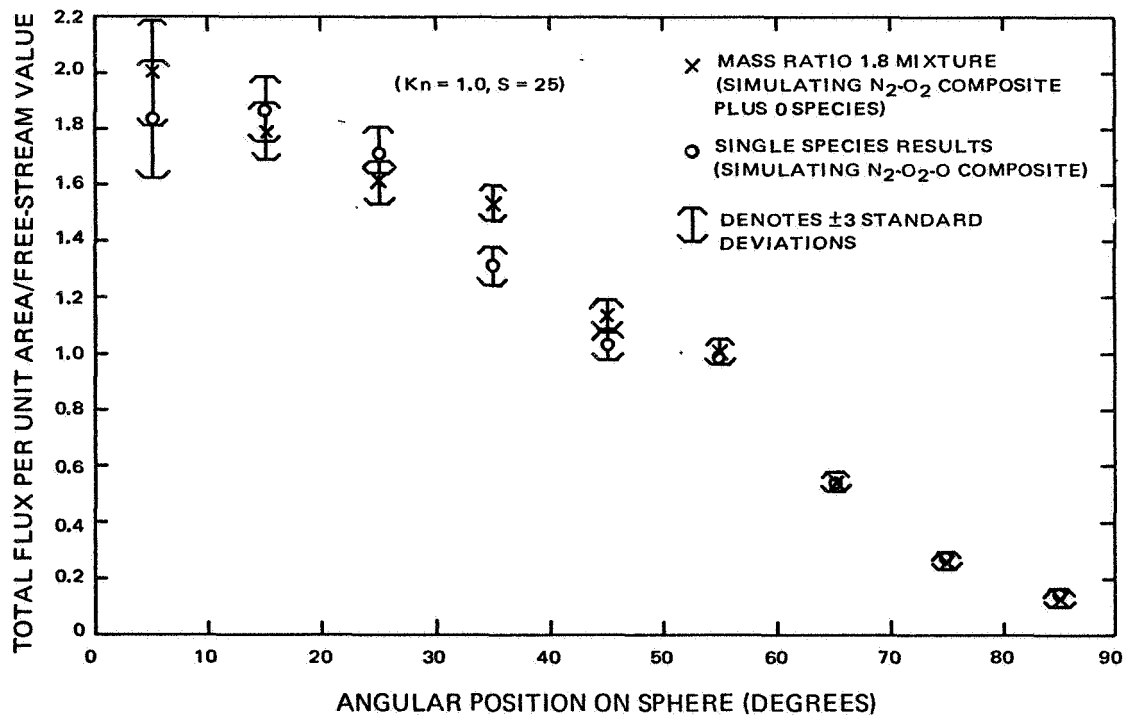

Figure 8.   Total Body Flux vs Angle for Composite Gas Simulation

SECTION IV

CONCLUSIONS

The primary objectives of this study were:

(1) To reorganize, generalize, and document the two-dimensional two-fluid program;

(2) To determine the feasibility of extending the program to more general situations including the three-dimensional multiple-fluid case;

(3) To construct a three-dimensional internal flow program compatible with the external flow program; and

(4) To examine techniques for synthesizing a single gas from two or more different gases and develop a technique for handling a trace gas.

These objectives have all been achieved, including considerable programming for the generalized three-dimensional two-fluid case.

The reorganization of the program has greatly improved its efficiency and ease of handling, as well as its understandability to persons who will not have had previous exposure to it. The geometry and reflection generalizations greatly simplify the program and provide maximum adaptability to a wide range of situations. The documentation provides to new users a sequential description of the program operating procedure.

The generalized three-dimensional program is an obvious extension of the successful two-dimensional program. It will provide the user with the ability to examine physical situations without requiring conditions to be extensively idealized. The availability of the IBM360-91 and -95 computers assures sufficient speed and storage to make the three-dimensional program feasible. Programming is well-underway for this case, and it is recommended that this program be completed.

The internal flow program can accommodate off-axis as well as on-axis flow, thus making it three-dimensional. As in the case of the external flow program, the geometry is limited to a finite number of connected sections with a common symmetry axis. It would be most desirable for the distribution function at the entrance to the cavity to be provided directly from the external flow program. However, the sample sizes are very small for average running times since the

approximately 1000 to 3000-sample particles striking the body segment have to be divided into velocity space cells. Thus, the sample in each velocity space cell is greatly reduced, or conversely, in order to increase such samples to reasonable values, the running time would have to be greatly increased. Additional techniques for coupling the external flow program body distribution to the internal flow program (requiring only small computer running times) are recommended for further study.

A prototype synthetic gas, composed first of molecular oxygen and nitrogen with atomic oxygen as the second specie, and then of the first two plus atomic oxygen all as a single gas was tested. The body flux parameters for the two cases were well-within three standard deviations of each other over most of the forward portion of the sphere. (Chemical effects were not considered.) For the study of trace constituents, it appears feasible to use the composite gas (N_2+O_2+O) as the main constituent and the trace gas (e. g. , helium or argon) as the second specie.

The physically significant results of this study are as follows:

(1) A large increase in density at and near the stagnation point (as high as 60 times the free-stream value for a Knudsen number of one). Accompanying the higher density will be an increased flux to the body. Measurement of this flux can lead to an erroneous impression of free-stream values. The incoming particle energies and momenta will also be greatly modified by the multiple collisions they experience as they approach the body, making it difficult to determine ambient conditions unless interaction effects are properly accounted for. Neglecting the interaction effect can result in gross underestimates of the local density values on the front of the vehicle.

(2) A pronounced depletion of the light particle flux, compared to the heavy, over the forward portion of the vehicle, especially near the stagnation point. (The ratio of the number of heavies to the number of lights gets very much larger than the free-stream value.) A preliminary physical interpretation of the basis for this effect is that the heavy particles have a greater persistence of velocity than the lights. In the stagnation region during particle-particle collisions, the lights will leave in random directions following collisions with the heavies, thereby having a higher probability of leaving this region. Again, considerable care must be taken in the interpretation of the data from flux-measuring sensors to relate local measurements to actual free-stream conditions.

SECTION V

LIST OF REFERENCES

1. "Study of Flow Fields in the Transitional Regime and Their Effects Upon Aeronomy Measurements", Final Report for Low-Altitude Satellite Interaction Problem Investigation Study on Contract No. NAS5-11016, prepared by RCA and issued May 17, 1968.

2. Bird, G.A., "Shock Wave Structure in a Rigid Sphere Gas", Rarefied Gas Dynamics (ed. by J.H. de Leeuw), Academic Press, Vol. I, p. 216, New York, 1965.

3. Bird, G.A., AIAA Journal, Vol 4, p.55 (1966).

4. Low-Altitude Satellite Interaction Problem Investigation, Program Report, prepared by RCA for NASA on Contract No. NAS5-11145, issued Nov. 1, 1968.

5. CIRA 1965.

6. Hughes, P.C., and de Leeuw, J.H., "Theory for the Free Molecule Impact Probe at an Angle of Attack", Rarefied Gas Dynamics, Academic Press, Supplement 3, Vol. I, p. 653, New York, 1965.